Lecture 6
Estimation

- Gaussian random vectors
- minimum mean-square estimation (MMSE)
- MMSE with linear measurements
- relation to least-squares, pseudo-inverse

Gaussian random vectors

random vector $x \in \mathbf{R}^n$ is *Gaussian* if it has density

$$p_x(v) = (2\pi)^{-n/2}(\det\Sigma)^{-1/2}\exp\left(-\frac{1}{2}(v-\bar{x})^T\Sigma^{-1}(v-\bar{x})\right),$$

for some $\Sigma = \Sigma^T > 0$, $\bar{x} \in \mathbf{R}^n$

- denoted $x \sim \mathcal{N}(\bar{x}, \Sigma)$
- $\bar{x} \in \mathbf{R}^n$ is the *mean* or *expected* value of x, $i.e.$,

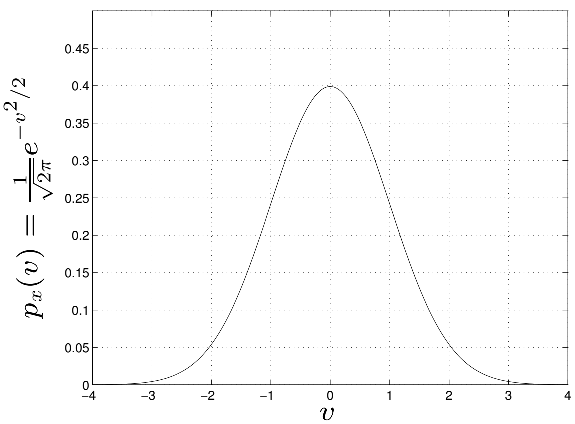
$$\bar{x} = \mathbf{E}\,x = \int v p_x(v)dv$$

- $\Sigma = \Sigma^T > 0$ is the *covariance* matrix of x, $i.e.$,

$$\Sigma \quad = \quad \mathbf{E}(x-\bar{x})(x-\bar{x})^T$$

$$\begin{aligned} &= \mathbf{E}\, xx^T - \bar{x}\bar{x}^T \\ &= \int (v-\bar{x})(v-\bar{x})^T p_x(v)\,dv \end{aligned}$$

density for $x \sim \mathcal{N}(0,1)$:



- mean and variance of scalar random variable x_i are

$$\mathbf{E}\, x_i = \bar{x}_i, \quad \mathbf{E}(x_i - \bar{x}_i)^2 = \Sigma_{ii}$$

  hence standard deviation of x_i is $\sqrt{\Sigma_{ii}}$

- covariance between x_i and x_j is $\mathbf{E}(x_i - \bar{x}_i)(x_j - \bar{x}_j) = \Sigma_{ij}$
- correlation coefficient between x_i and x_j is $\rho_{ij} = \dfrac{\Sigma_{ij}}{\sqrt{\Sigma_{ii}\Sigma_{jj}}}$
- mean (norm) square deviation of x from $\bar{x}$ is

$$\mathbf{E}\,\|x - \bar{x}\|^2 = \mathbf{E}\,\mathbf{Tr}(x-\bar{x})(x-\bar{x})^T = \mathbf{Tr}\,\Sigma = \sum_{i=1}^n \Sigma_{ii}$$

  (using $\mathbf{Tr}\,AB = \mathbf{Tr}\,BA$)

example: $x \sim \mathcal{N}(0, I)$ means x_i are independent identically distributed (IID) $\mathcal{N}(0,1)$ random variables

Confidence ellipsoids

$p_x(v)$ is constant for $(v-\bar{x})^T\Sigma^{-1}(v-\bar{x})=\alpha$, *i.e.*, on the surface of ellipsoid

$$\mathcal{E}_\alpha=\{v \mid (v-\bar{x})^T\Sigma^{-1}(v-\bar{x})\leq\alpha\}$$

thus $\bar{x}$ and Σ determine shape of density

can interpret $\mathcal{E}_\alpha$ as *confidence ellipsoid* for x:

the nonnegative random variable $(x-\bar{x})^T\Sigma^{-1}(x-\bar{x})$ has a χ_n^2 distribution, so $\mathbf{Prob}(x\in\mathcal{E}_\alpha)=F_{\chi_n^2}(\alpha)$ where $F_{\chi_n^2}$ is the CDF

some good approximations:

- $\mathcal{E}_n$ gives about 50% probability
- $\mathcal{E}_{n+2\sqrt{n}}$ gives about 90% probability

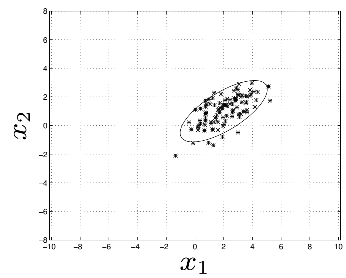
geometrically:

- mean $\bar{x}$ gives center of ellipsoid
- semiaxes are $\sqrt{\alpha\lambda_i}u_i$, where u_i are (orthonormal) eigenvectors of Σ with eigenvalues λ_i

example: $x \sim \mathcal{N}(\bar{x}, \Sigma)$ with $\bar{x} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$, $\Sigma = \begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix}$

- x_1 has mean 2, std. dev. $\sqrt{2}$
- x_2 has mean 1, std. dev. 1
- correlation coefficient between x_1 and x_2 is $\rho = 1/\sqrt{2}$
- $\mathbf{E}\,\|x - \bar{x}\|^2 = 3$

90% confidence ellipsoid corresponds to $\alpha = 4.6$:



(here, 91 out of 100 fall in $\mathcal{E}_{4.6}$)

Affine transformation

suppose $x \sim \mathcal{N}(\bar{x}, \Sigma_x)$

consider affine transformation of x:

$$z = Ax + b,$$

where $A \in \mathbf{R}^{m \times n}$, $b \in \mathbf{R}^m$

then z is Gaussian, with mean

$$\mathbf{E}\,z = \mathbf{E}(Ax + b) = A\,\mathbf{E}\,x + b = A\bar{x} + b$$

and covariance

$$\begin{aligned} \Sigma_z &= \mathbf{E}(z - \bar{z})(z - \bar{z})^T \\ &= \mathbf{E}\,A(x - \bar{x})(x - \bar{x})^T A^T \\ &= A\Sigma_x A^T \end{aligned}$$

examples:

- if $w \sim \mathcal{N}(0, I)$ then $x = \Sigma^{1/2} w + \bar{x}$ is $\mathcal{N}(\bar{x}, \Sigma)$

  useful for simulating vectors with given mean and covariance

- conversely, if $x \sim \mathcal{N}(\bar{x}, \Sigma)$ then $z = \Sigma^{-1/2}(x - \bar{x})$ is $\mathcal{N}(0, I)$

  (normalizes & decorrelates)

suppose $x \sim \mathcal{N}(\bar{x}, \Sigma)$ and $c \in \mathbf{R}^n$

scalar $c^T x$ has mean $c^T \bar{x}$ and variance $c^T \Sigma c$

thus (unit length) direction of minimum variability for x is u, where

$$\Sigma u = \lambda_{\min} u, \quad \|u\| = 1$$

standard deviation of $u_n^T x$ is $\sqrt{\lambda_{\min}}$

(similarly for maximum variability)

Degenerate Gaussian vectors

it is convenient to allow Σ to be singular (but still $\Sigma = \Sigma^T \geq 0$)

(in this case density formula obviously does not hold)

meaning: in some directions x is not random at all

write Σ as

$$\Sigma = [Q_+ \ Q_0] \begin{bmatrix} \Sigma_+ & 0 \\ 0 & 0 \end{bmatrix} [Q_+ \ Q_0]^T$$

where $Q = [Q_+ \ Q_0]$ is orthogonal, $\Sigma_+ > 0$

- columns of Q_0 are orthonormal basis for $\mathcal{N}(\Sigma)$
- columns of Q_+ are orthonormal basis for $\mathrm{range}(\Sigma)$

then $Q^T x = [z^T \ w^T]^T$, where

- $z \sim \mathcal{N}(Q_+^T \bar{x}, \Sigma_+)$ is (nondegenerate) Gaussian (hence, density formula holds)
- $w = Q_0^T \bar{x} \in \mathbf{R}^n$ is not random

  ($Q_0^T x$ is called *deterministic component* of x)

Linear measurements

linear measurements with noise:

$$y = Ax + v$$

- $x \in \mathbf{R}^n$ is what we want to measure or estimate
- $y \in \mathbf{R}^m$ is measurement
- $A \in \mathbf{R}^{m \times n}$ characterizes sensors or measurements
- v is sensor noise

common assumptions:

- $x \sim \mathcal{N}(\bar{x}, \Sigma_x)$
- $v \sim \mathcal{N}(\bar{v}, \Sigma_v)$
- x and v are independent

- $\mathcal{N}(\bar{x}, \Sigma_x)$ is the *prior distribution* of x (describes initial uncertainty about x)
- $\bar{v}$ is noise *bias* or *offset* (and is usually 0)
- Σ_v is noise *covariance*

thus

$$\begin{bmatrix} x \\ v \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \bar{x} \\ \bar{v} \end{bmatrix}, \begin{bmatrix} \Sigma_x & 0 \\ 0 & \Sigma_v \end{bmatrix}\right)$$

using

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} I & 0 \\ A & I \end{bmatrix} \begin{bmatrix} x \\ v \end{bmatrix}$$

we can write

$$\mathbf{E} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} \bar{x} \\ A\bar{x} + \bar{v} \end{bmatrix}$$

and

$$\begin{aligned} \mathbf{E} \begin{bmatrix} x - \bar{x} \\ y - \bar{y} \end{bmatrix} \begin{bmatrix} x - \bar{x} \\ y - \bar{y} \end{bmatrix}^T &= \begin{bmatrix} I & 0 \\ A & I \end{bmatrix} \begin{bmatrix} \Sigma_x & 0 \\ 0 & \Sigma_v \end{bmatrix} \begin{bmatrix} I & 0 \\ A & I \end{bmatrix}^T \\ &= \begin{bmatrix} \Sigma_x & \Sigma_x A^T \\ A\Sigma_x & A\Sigma_x A^T + \Sigma_v \end{bmatrix} \end{aligned}$$

covariance of measurement y is $A\Sigma_x A^T + \Sigma_v$

- $A\Sigma_x A^T$ is ‘signal covariance’
- Σ_v is ‘noise covariance’

Minimum mean-square estimation

suppose $x \in \mathbf{R}^n$ and $y \in \mathbf{R}^m$ are random vectors (not necessarily Gaussian)

we seek to estimate x given y

thus we seek a function $\phi : \mathbf{R}^m \to \mathbf{R}^n$ such that $\hat{x} = \phi(y)$ is near x

one common measure of nearness: mean-square error,

$$\mathbf{E}\,\|\phi(y) - x\|^2$$

minimum mean-square estimator (MMSE) ϕ_{mmse} minimizes this quantity

general solution: $\phi_{\mathrm{mmse}}(y) = \mathbf{E}(x|y)$, $i.e.$, the conditional expectation of x given y

MMSE for Gaussian vectors

now suppose $x \in \mathbf{R}^n$ and $y \in \mathbf{R}^m$ are jointly Gaussian:

$$\begin{bmatrix} x \\ y \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \bar{x} \\ \bar{y} \end{bmatrix}, \begin{bmatrix} \Sigma_x & \Sigma_{xy} \\ \Sigma_{xy}^T & \Sigma_y \end{bmatrix} \right)$$

(after alot of algebra) the conditional density is

$$p_{x|y}(v|y) = (2\pi)^{-n/2}(\det\Lambda)^{-1/2}\exp\left(-\frac{1}{2}(v-w)^T\Lambda^{-1}(v-w)\right),$$

where

$$\Lambda = \Sigma_x - \Sigma_{xy}\Sigma_y^{-1}\Sigma_{xy}^T, \quad w = \bar{x} + \Sigma_{xy}\Sigma_y^{-1}(y - \bar{y})$$

hence MMSE estimator ($i.e.$, conditional expectation) is

$$\hat{x} = \phi_{\mathrm{mmse}}(y) = \mathbf{E}(x|y) = \bar{x} + \Sigma_{xy}\Sigma_y^{-1}(y - \bar{y})$$

ϕ_{mmse} is an affine function

MMSE estimation error, $\hat{x} - x$, is a Gaussian random vector

$$\hat{x} - x \;\sim\; \mathcal{N}(0, \Sigma_x - \Sigma_{xy}\Sigma_y^{-1}\Sigma_{xy}^T)$$

note that

$$\Sigma_x - \Sigma_{xy}\Sigma_y^{-1}\Sigma_{xy}^T \leq \Sigma_x$$

$i.e.$, covariance of estimation error is always less than prior covariance of x

Best linear unbiased estimator

estimator

$$\hat{x} = \phi_{\mathrm{blu}}(y) = \bar{x} + \Sigma_{xy}\Sigma_y^{-1}(y - \bar{y})$$

makes sense when x, y aren't jointly Gaussian

this estimator

- is *unbiased*, $i.e.$, $\mathbf{E}\,\hat{x} = \mathbf{E}\,x$
- often works well
- is widely used
- has minimum mean square error among all *affine* estimators

sometimes called *best linear unbiased* estimator

MMSE with linear measurements

consider specific case

$$y = Ax + v, \quad x \sim \mathcal{N}(\bar{x}, \Sigma_x), \quad v \sim \mathcal{N}(\bar{v}, \Sigma_v),$$

x, v independent

MMSE of x given y is affine function

$$\hat{x} = \bar{x} + B(y - \bar{y})$$

where $B = \Sigma_x A^T (A \Sigma_x A^T + \Sigma_v)^{-1}$, $\bar{y} = A\bar{x} + \bar{v}$

intepretation:

- $\bar{x}$ is our best prior guess of x (before measurement)
- $y - \bar{y}$ is the discrepancy between what we actually measure (y) and the expected value of what we measure ($\bar{y}$)

- estimator modifies prior guess by B times this discrepancy
- estimator blends prior information with measurement
- B gives *gain* from *observed discrepancy* to *estimate*
- B is small if noise term Σ_v in 'denominator' is large

MMSE error with linear measurements

MMSE estimation error, $\tilde{x} = \hat{x} - x$, is Gaussian with zero mean and covariance

$$\Sigma_{\rm est} = \Sigma_x - \Sigma_x A^T (A\Sigma_x A^T + \Sigma_v)^{-1} A\Sigma_x$$

- $\Sigma_{\rm est} \leq \Sigma_x$, *i.e.*, measurement always decreases uncertainty about x
- difference $\Sigma_x - \Sigma_{\rm est}$ gives *value* of measurement y in estimating x
- *e.g.*, $(\Sigma_{\rm est\ \it ii}/\Sigma_{x\ ii})^{1/2}$ gives fractional decrease in uncertainty of x_i due to measurement

note: error covariance $\Sigma_{\rm est}$ can be determined *before* measurement y is made!

to evaluate $\Sigma_{\rm est}$, only need to know

- A (which characterizes sensors)
- prior covariance of x (*i.e.*, Σ_x)
- noise covariance (*i.e.*, Σ_v)

you *do not* need to know the measurement y (or the means $\bar{x}$, $\bar{v}$)

useful for *experiment design* or *sensor selection*

Information matrix formulas

we can write estimator gain matrix as

$$\begin{aligned} B &= \Sigma_x A^T (A\Sigma_x A^T + \Sigma_v)^{-1} \\ &= \left(A^T\Sigma_v^{-1}A + \Sigma_x^{-1}\right)^{-1} A^T\Sigma_v^{-1} \end{aligned}$$

- $n \times n$ inverse instead of $m \times m$
- Σ_x^{-1}, Σ_v^{-1} sometimes called *information matrices*

corresponding formula for estimator error covariance:

$$\begin{aligned} \Sigma_{\text{est}} &= \Sigma_x - \Sigma_x A^T (A\Sigma_x A^T + \Sigma_v)^{-1} A\Sigma_x \\ &= \left(A^T\Sigma_v^{-1}A + \Sigma_x^{-1}\right)^{-1} \end{aligned}$$

can interpret $\Sigma_{\text{est}}^{-1} = \Sigma_x^{-1} + A^T\Sigma_v^{-1}A$ as:

posterior information matrix $(\Sigma_{\text{est}}^{-1})$
$=$ prior information matrix (Σ_x^{-1})
$+$ information added by measurement $(A^T\Sigma_v^{-1}A)$

proof: multiply

$$\Sigma_x A^T (A\Sigma_x A^T + \Sigma_v)^{-1} \stackrel{?}{=} \left(A^T\Sigma_v^{-1}A + \Sigma_x^{-1}\right)^{-1} A^T\Sigma_v^{-1}$$

on left by $(A^T\Sigma_v^{-1}A + \Sigma_x^{-1})$ and on right by $(A\Sigma_x A^T + \Sigma_v)$ to get

$$(A^T\Sigma_v^{-1}A + \Sigma_x^{-1})\Sigma_x A^T \stackrel{?}{=} A^T\Sigma_v^{-1}(A\Sigma_x A^T + \Sigma_v)$$

which is true

Relation to regularized least-squares

suppose $\bar{x} = 0$, $\bar{v} = 0$, $\Sigma_x = \alpha^2 I$, $\Sigma_v = \beta^2 I$

estimator is $\hat{x} = By$ where

$$\begin{aligned} B &= \left(A^T\Sigma_v^{-1}A + \Sigma_x^{-1}\right)^{-1} A^T\Sigma_v^{-1} \\ &= (A^TA + (\beta/\alpha)^2 I)^{-1}A^T \end{aligned}$$

. . . which corresponds to regularized least-squares

MMSE estimate $\hat{x}$ minimizes

$$\|Az - y\|^2 + (\beta/\alpha)^2\|z\|^2$$

over z

Example

navigation using range measurements to distant beacons

$$y = Ax + v$$

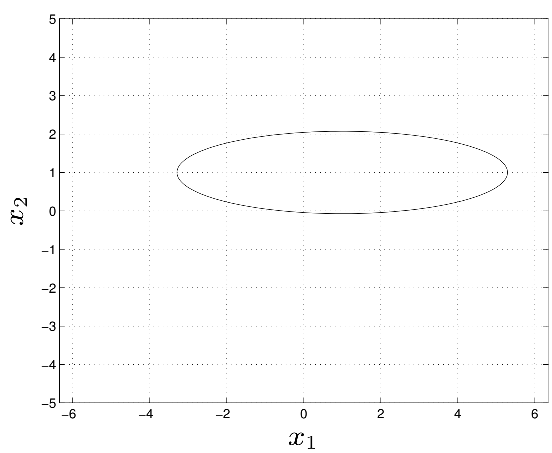
- $x \in \mathbf{R}^2$ is location
- y_i is range measurement to ith beacon
- v_i is range measurement error, IID $\mathcal{N}(0, 1)$
- ith row of A is unit vector in direction of ith beacon

prior distribution:

$$x \sim \mathcal{N}(\bar{x}, \Sigma_x), \quad \bar{x} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \Sigma_x = \begin{bmatrix} 2^2 & 0 \\ 0 & 0.5^2 \end{bmatrix}$$

x_1 has std. dev. 2; x_2 has std. dev. 0.5

90% confidence ellipsoid for prior distribution
$\{ \, x \mid (x - \bar{x})^T \Sigma_x^{-1} (x - \bar{x}) \le 4.6 \, \}$:



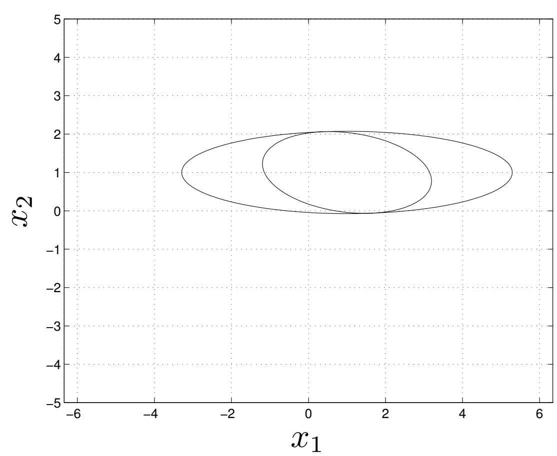
Case 1: one measurement, with beacon at angle $30°$

fewer measurements than variables, so combining prior information with measurement is critical

resulting estimation error covariance:

$$\Sigma_{\text{est}} = \begin{bmatrix} 1.046 & -0.107 \\ -0.107 & 0.246 \end{bmatrix}$$

90% confidence ellipsoid for estimate $\hat{x}$: (and 90% confidence ellipsoid for x)



interpretation: measurement

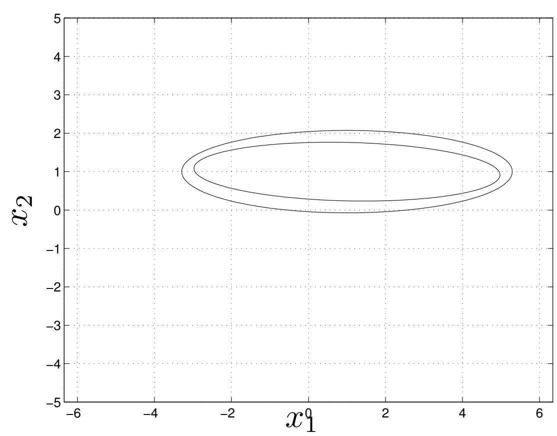
- yields essentially no reduction in uncertainty in x_2
- reduces uncertainty in x_1 by a factor about two

Case 2: 4 measurements, with beacon angles $80°,\ 85°,\ 90°,\ 95°$

resulting estimation error covariance:

$$\Sigma_{\rm est} = \begin{bmatrix} 3.429 & -0.074 \\ -0.074 & 0.127 \end{bmatrix}$$

90% confidence ellipsoid for estimate $\hat{x}$: (and 90% confidence ellipsoid for x)



interpretation: measurement yields

- little reduction in uncertainty in x_1
- small reduction in uncertainty in x_2